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Title: Numerical Simulation of Mixing Layers Involving Two Fluids of Different Densities

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Numerical Simulation of Mixing Layers Involving Two Fluids of Different Densities

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Variable-Density Turbulent Shear Layer

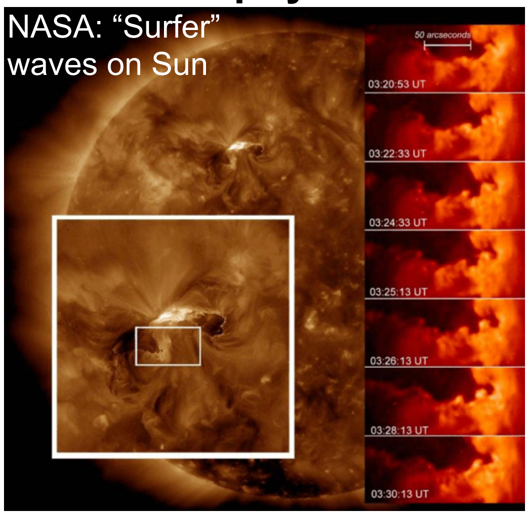
- **Mixing layer between two parallel streams of fluids with different velocities and densities; instability leads to turbulence**
- **Distinctive structures have long been observed to occur (Kelvin-Helmholtz instability)**

- **Shear is one of the principal mechanisms for generating turbulence; buoyancy has been extensively studied at LANL while shear has received much less attention**

Variable-Density Turbulent Shear Layer

- **Applications include:**

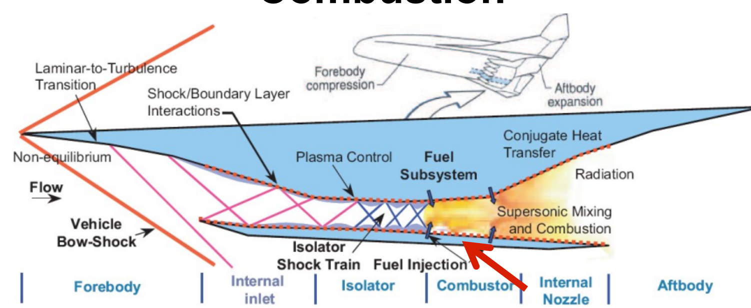
Astrophysics



Wind-wave Interaction

Pollutant Dispersion

Combustion



Scramjet, Stanford CTR (PSAAP project)

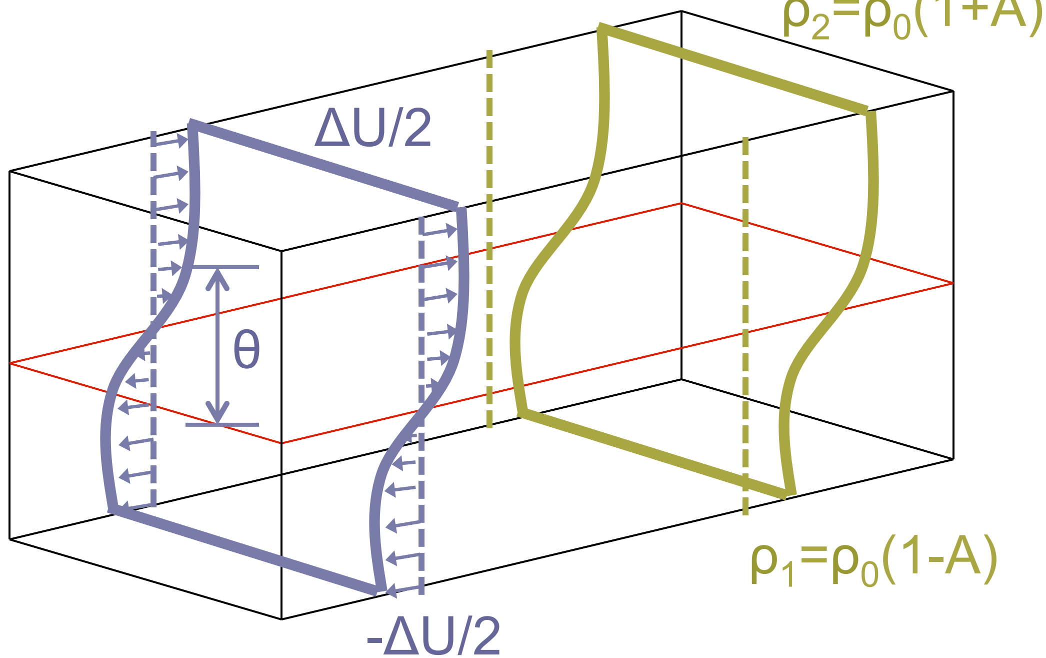
Variable-Density Turbulent Shear Layer

- **Open questions:**
  - How do variable-density effects affect mixing?
  - How do variable-density effects affect entrainment?
  - No studies focusing explicitly on variable-density effects (most studies consider high-speed flows; very difficult to separate effects of compressibility from effects of variable density)

Prototypical Flow

- **Simulation of many practical flows require turbulence models that include variable density effects**
  - Direct simulation not feasible for these cases → RANS
  - Most models do not account for variable density effects
  - BHR model developed at LANL
  - Models require testing and coefficients determined from DNS/experiment
- **Temporal mixing layer allows us to examine salient physics**
  - Simulated in periodic box (does not develop spatially)
  - DNS gives us control over initial conditions (disturbance); difficult with experiments

Prototypical Flow: Problem Description



- **Momentum-thickness Reynolds number $Re_\theta=(\theta)(\Delta U)/\nu$**
- **Atwood number $A=(\rho_2-\rho_1)/(\rho_2+\rho_1)$**
- **Constant viscosity ($\nu=\mu/\rho$)**

Variable-density turbulence

- **Mixing between fluids with very different densities: variable-density mixing.**
- **The equations describing the variable-density mixing between two incompressible fluids can be derived from the compressible Navier-Stokes equations with two ideal gases, by letting *P, T* → ∞ such that** $\rho_1 = P/(T\mathcal{R}W_1)$ **and** $\rho_2 = P/(T\mathcal{R}W_2)$ **remain constant.**

Continuity $$\rho_{,t} + (\rho u_j)_{,j} = 0$$

no buoyant effects

Momentum $$(\rho u_i)_{,t} + (\rho u_i u_j)_{,j} = -p_{,i} + \mu(u_{i,j} + u_{j,i} - 2/3\delta_{ij}u_{k,k})_{,j} + \cancel{\rho g_i}$$

Divergence condition $$u_{j,j} = -\mathcal{D}Ln(\rho)_{,jj}$$

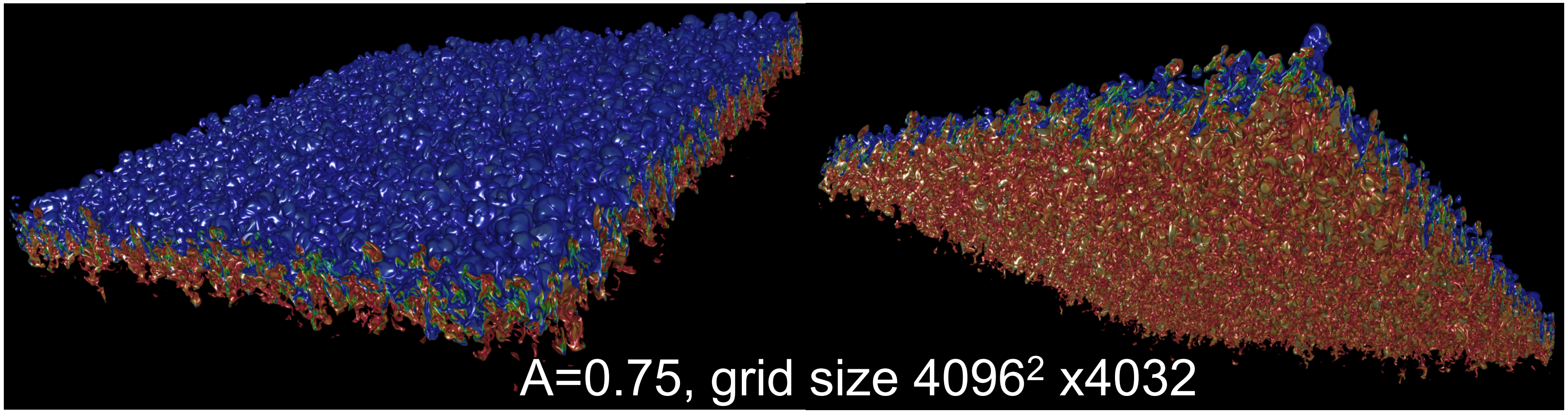
- **Same equations as those used for Rayleigh-Taylor studies (but no buoyancy)**
- **Boussinesq approximation (only retaining density terms directly related to gravity) would eliminate all density effects for mixing layer in this case**

DNS of Prototypical Variable Density Shear-Driven Mixing Layer

- **DNS: fully resolve all dynamically relevant scales → important for obtaining reliable statistics to be used for models**
- **Requires numerical treatment that accurately represents variable density effects**
- **Very large computational problems are necessary**
  - Reynolds number (range of scales)
  - Long wavelengths; Mode pairing (necessary physics of problem)

Simulation Code: CFDNS

- **Code used: CFDNS (Livescu et al. LA-CC-09-100)**
- **Has been applied to Rayleigh-Taylor (variable-density, buoyancy-driven) instability**



- **3-D simulations (up to 4096^2 x 4032) performed on Dawn, LLNL; Jaguar, ORNL; Cielo, LANL; and Sequoia, LLNL up to 250,000 compute cores**

CFDNS: Numerical Methods

- For this problem, mixed FFTs - 6th order compact finite differences (slip walls represent boundaries of fluid layers, periodic in horizontal directions).
- Pressure projection method with a variable time stepping third order Adams-Bashforth-Moulton for time advancement.
- Main difficulty: Density variations lead to a variable coefficient Poisson equation (Livescu and Ristorcelli, J. Fluid Mech. 2007).

$$\nabla \bullet \left(\frac{\nabla p}{\rho} \right) = F(\vec{x}); \qquad \frac{\nabla p}{\rho} \bullet \vec{n} = \frac{\rho^n \vec{u}^n}{\rho^{n+1}} \bullet \vec{n} \,|_\Gamma$$

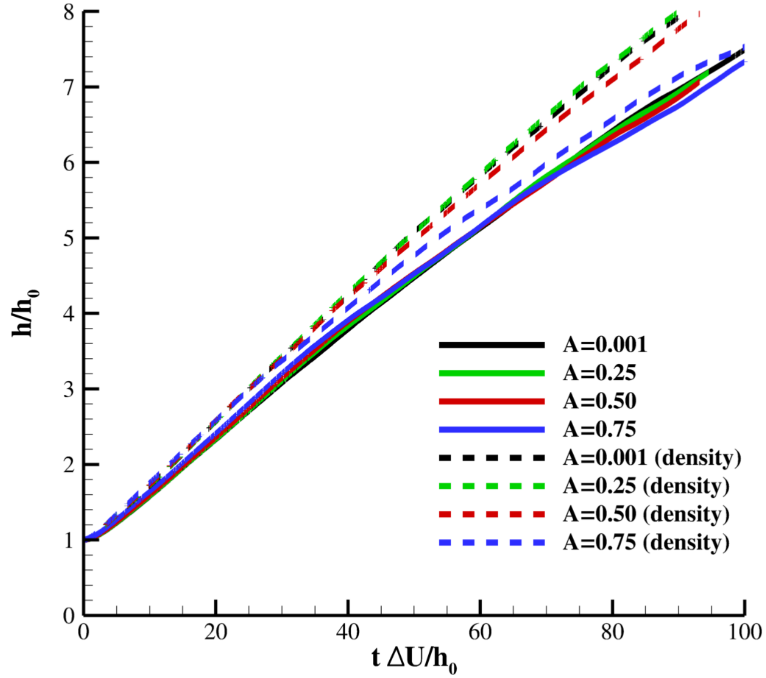
- Closed form solution for the gradient component, **q**, of $\nabla p / \rho$, responsible for mass conservation
- Iterative solver for the curl component, **Q**, of $\nabla p / \rho$, related to the baroclinic production of vorticity (Livescu and Ristorcelli, J. Fluid Mech. 2007 and Chung and Pullin, J. Fluid Mech. 2010).

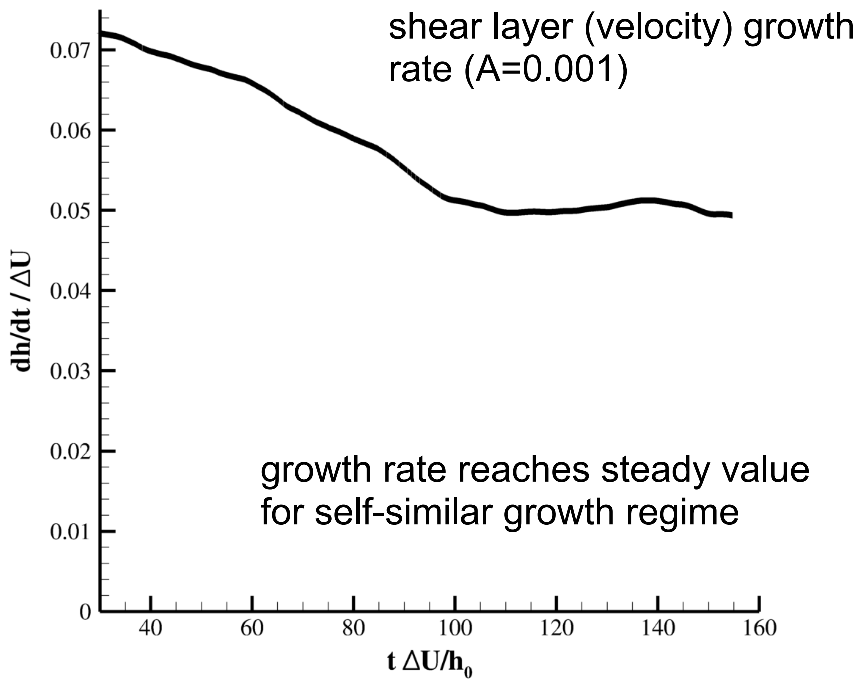
$$\nabla^2 \vec{q} = F(\vec{x}); \qquad \nabla q \bullet \vec{n} = \frac{\rho^n \vec{u}^n}{\rho^{n+1}} \bullet \vec{n} \,|_\Gamma$$

$$\nabla^2 \vec{Q} = \nabla \times \left[\nabla \ln \rho \times \left(\vec{Q} + \vec{q} \right) \right]; \qquad \vec{Q} \bullet \vec{n} = 0 \,|_\Gamma$$

Application of CFDNS to Variable Density Shear-Driven Mixing Layer

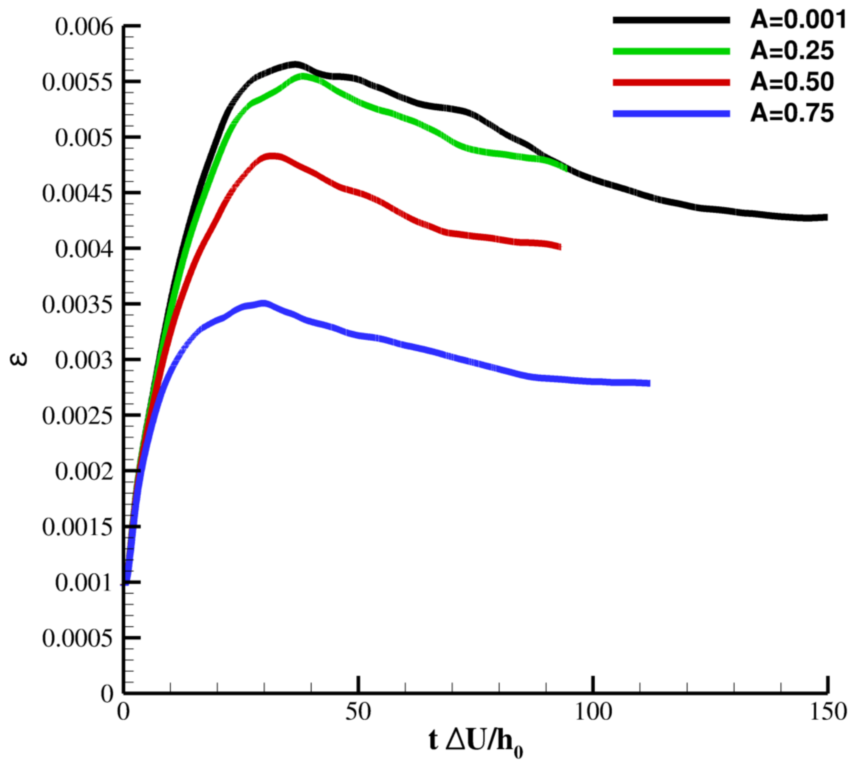
- **Preliminary results:**
- **h defined as width between points at which area-averaged streamwise velocity is at 10% and 90% of total velocity difference ΔU (and similar for density difference between streams)**





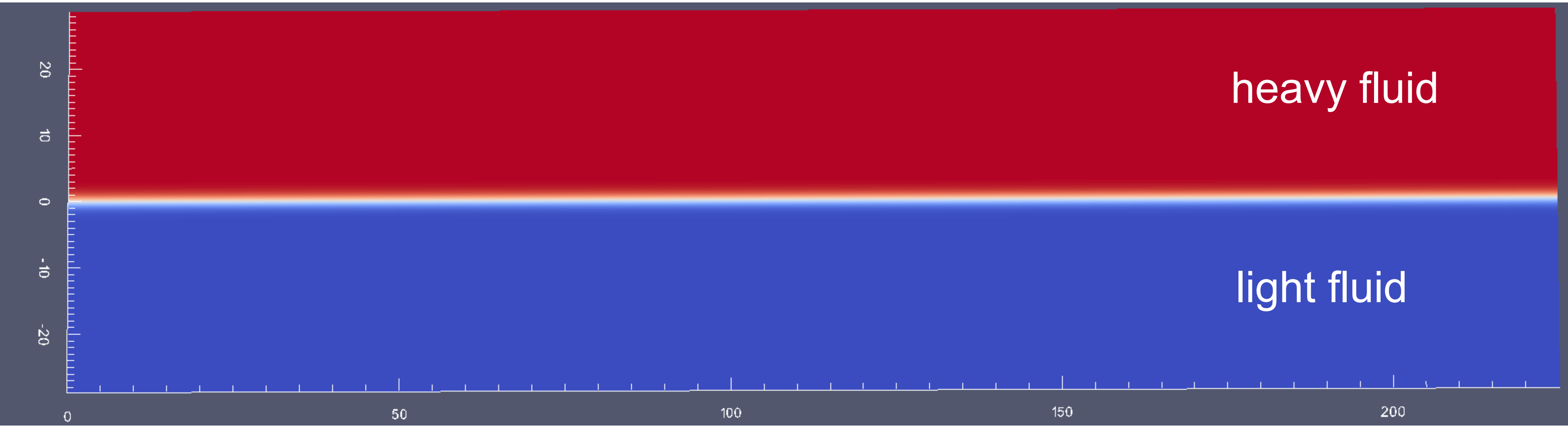
- **Early time growth of velocity and density similar for all A; at later times, density growth is slower for large A while velocity growth remains similar between all A**

Application of CFDNS to Variable Density Shear-Driven Mixing Layer



- Atwood number has significant effect on volume-integrated dissipation
- Approach constant values in self-similar growth regime

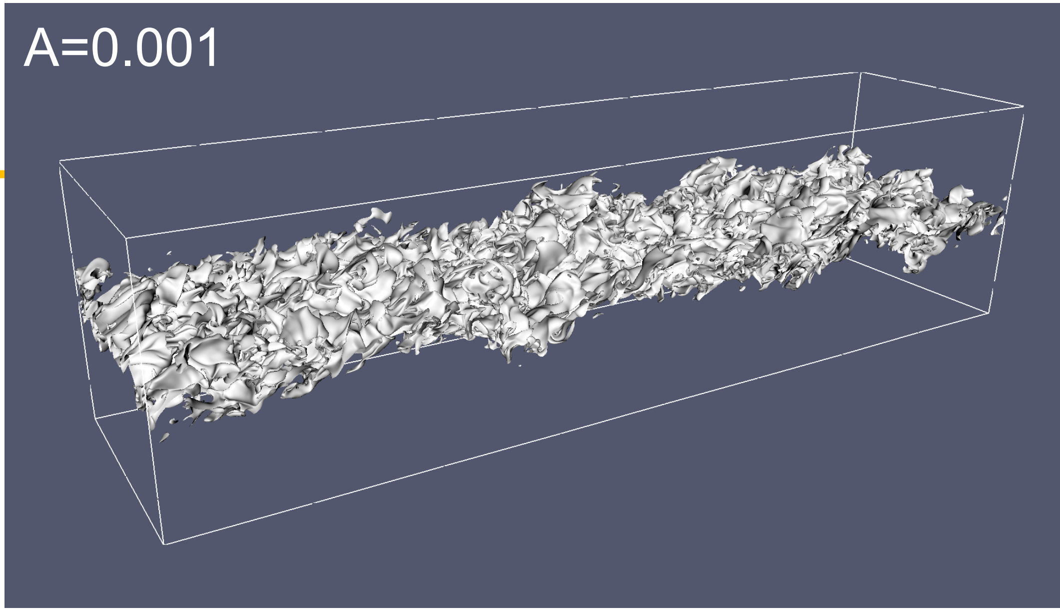
Initial Density Profile

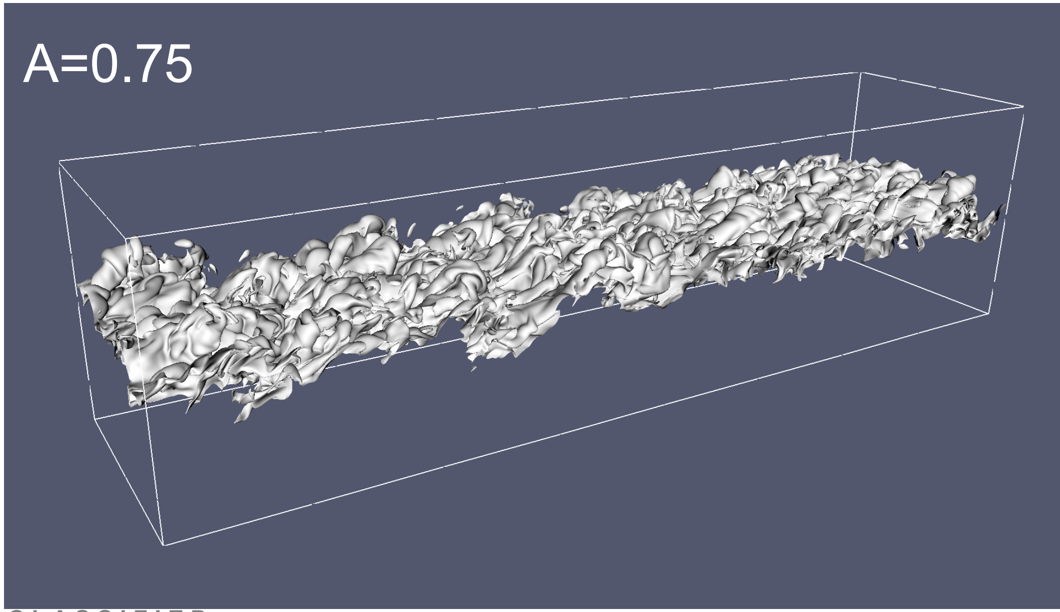


- No density perturbation; interface is flat sheet in 3D
- Density is a useful quantity for tracking mixing (by tracking the density interface)

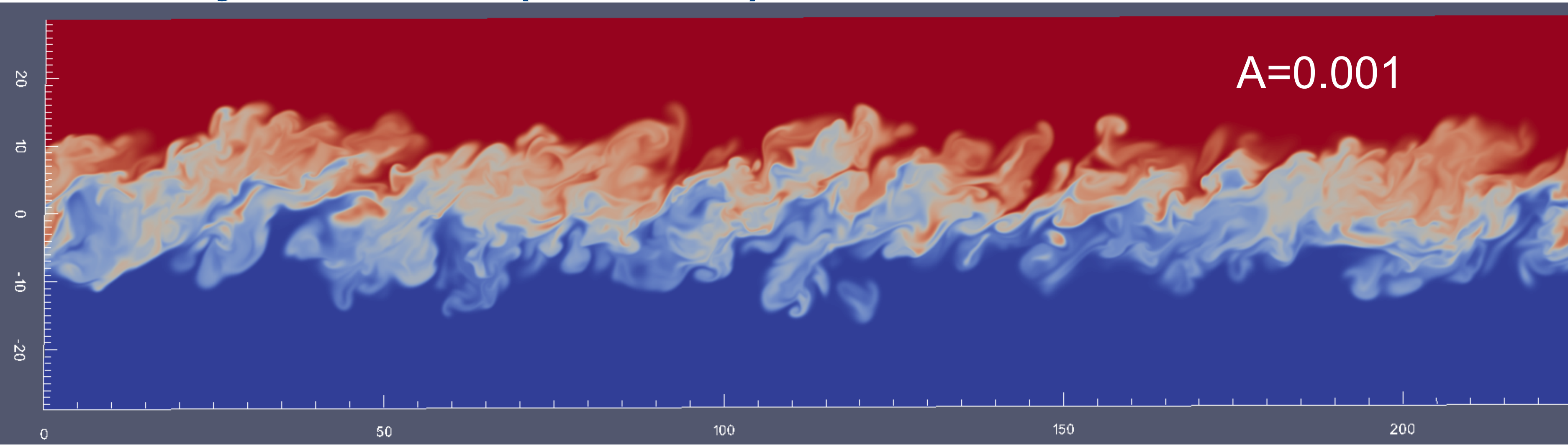
Density Contour Surfaces (late time)

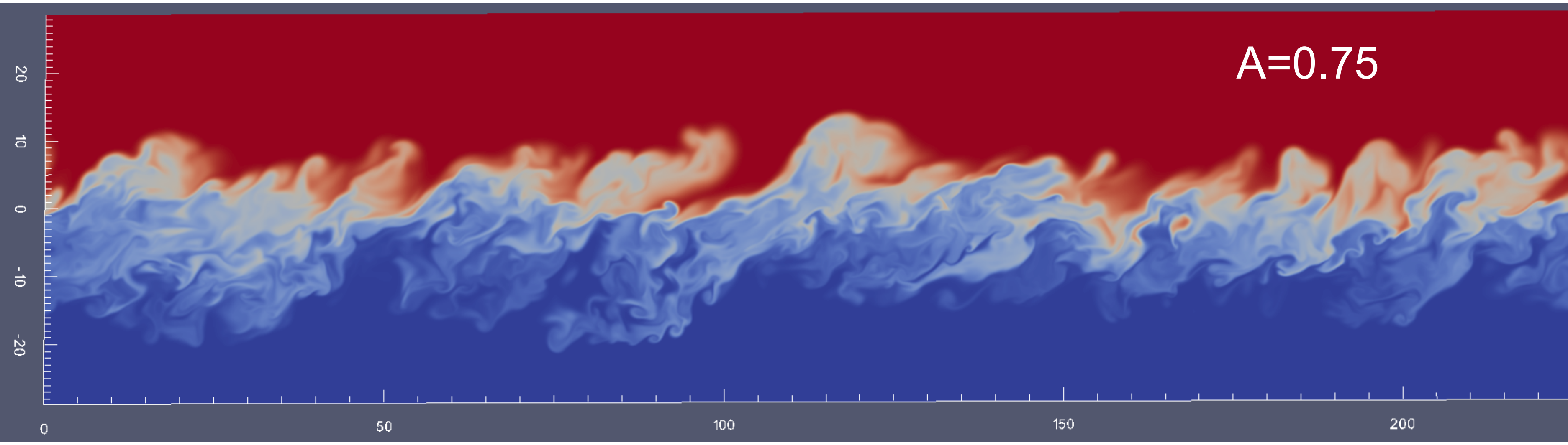
- Contours of density at center of initial interface ($\rho=\rho_0$)
- Evolved from initial flat sheet





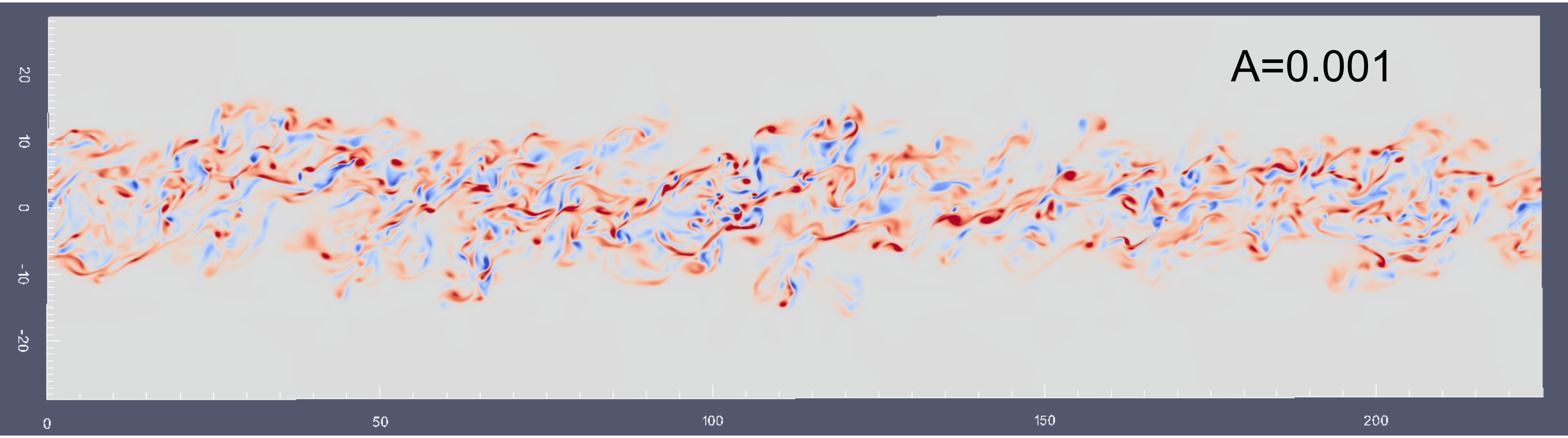
Density Contours (late time)

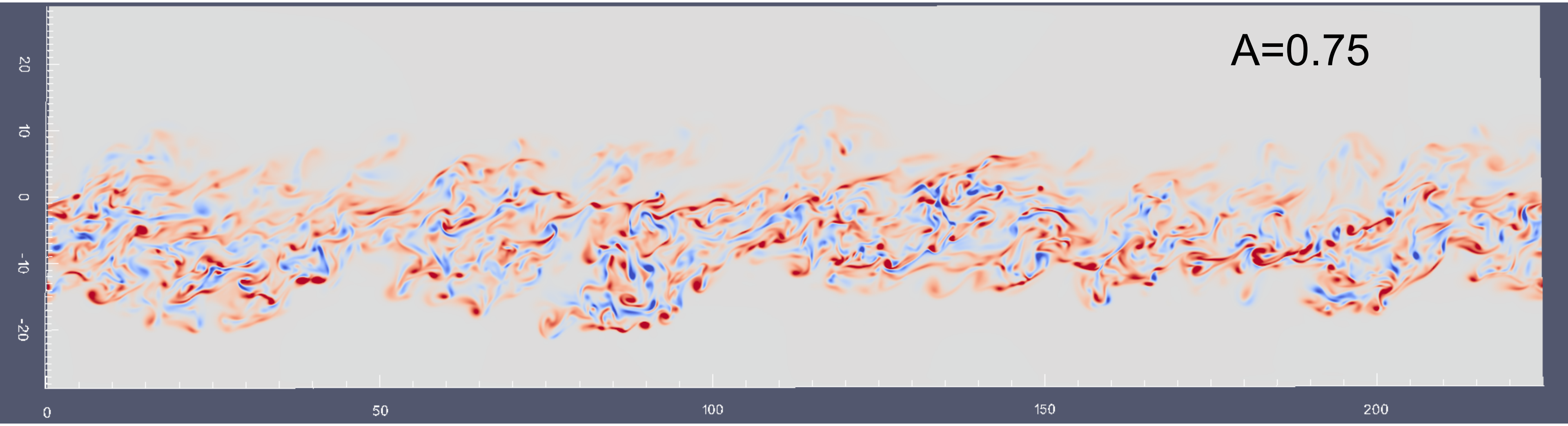




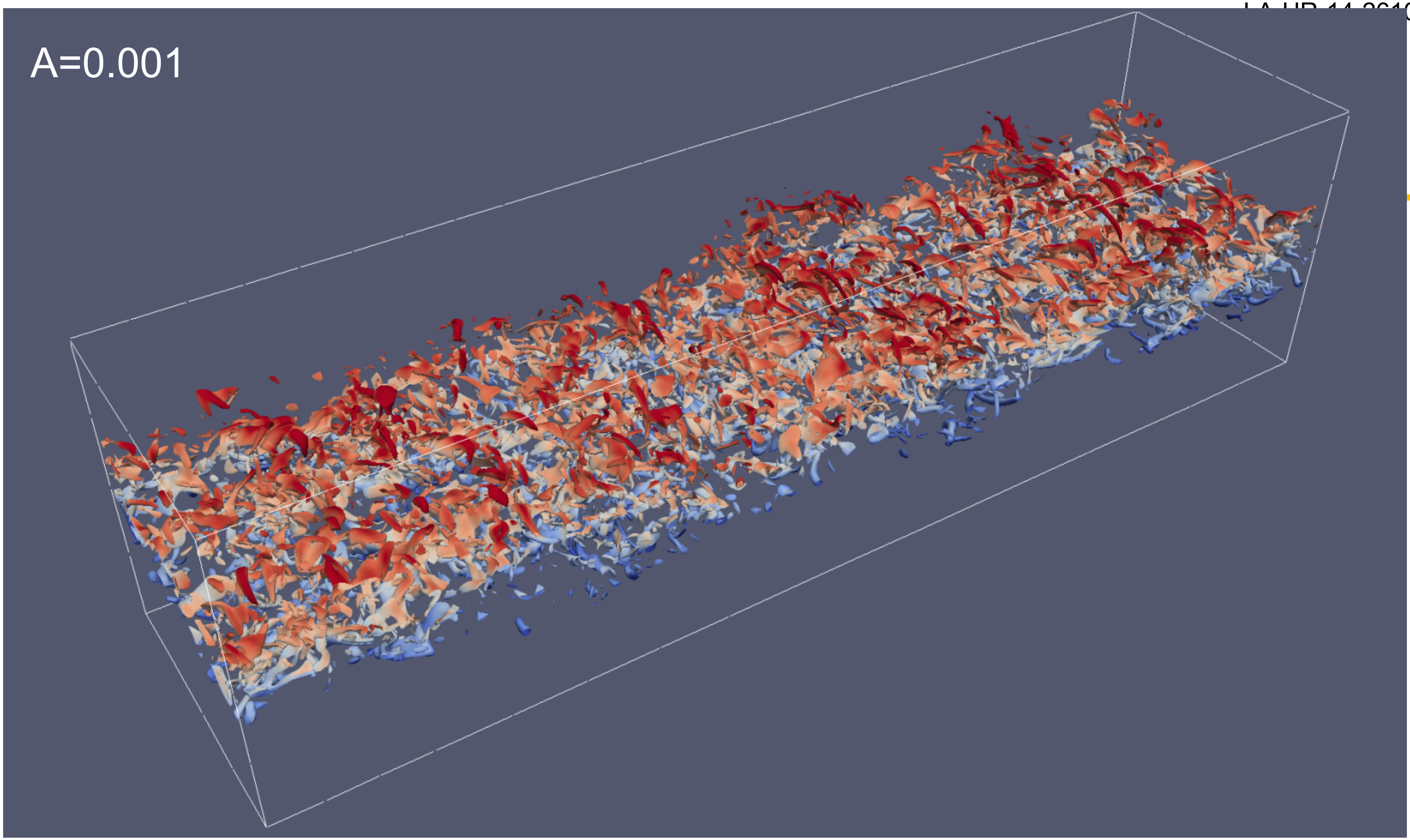
- **High Atwood number: layer is asymmetric; mixing penetrates deeper into the lower-density side; structures are finer relative to higher-density side**

Spanwise Vorticity Contours (late time)

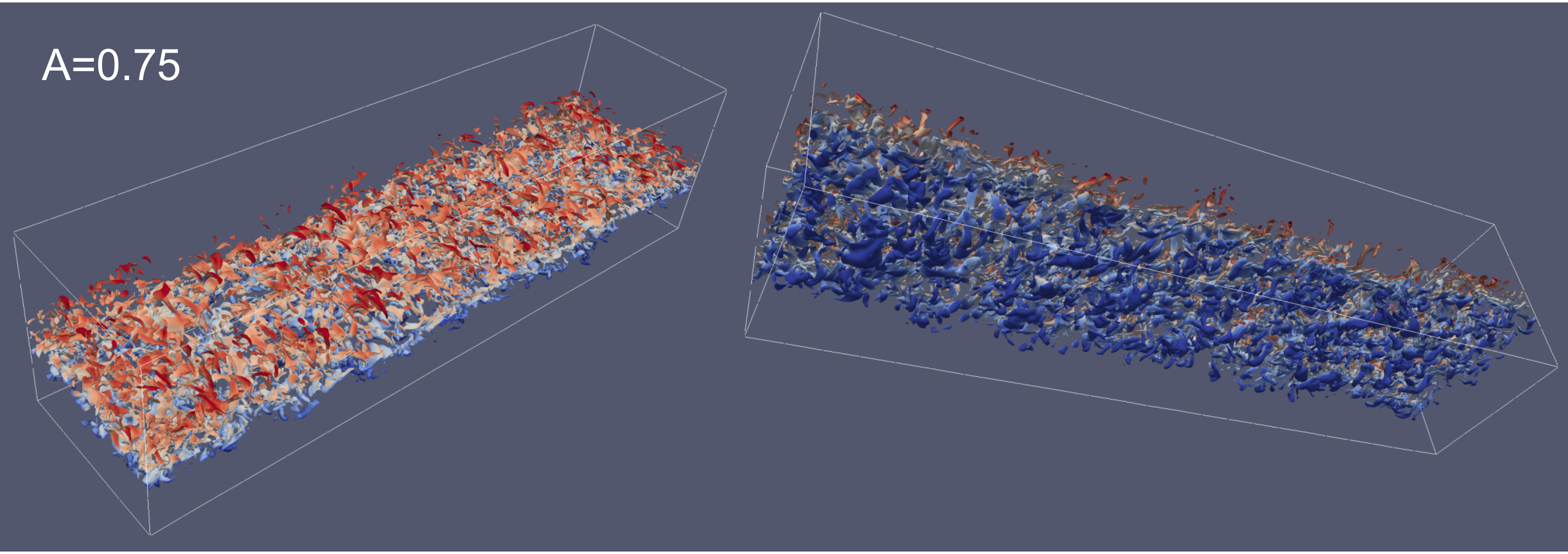




- **Growth of turbulent structures toward low-density fluid is similar to transport of density in high-Atwood number case**

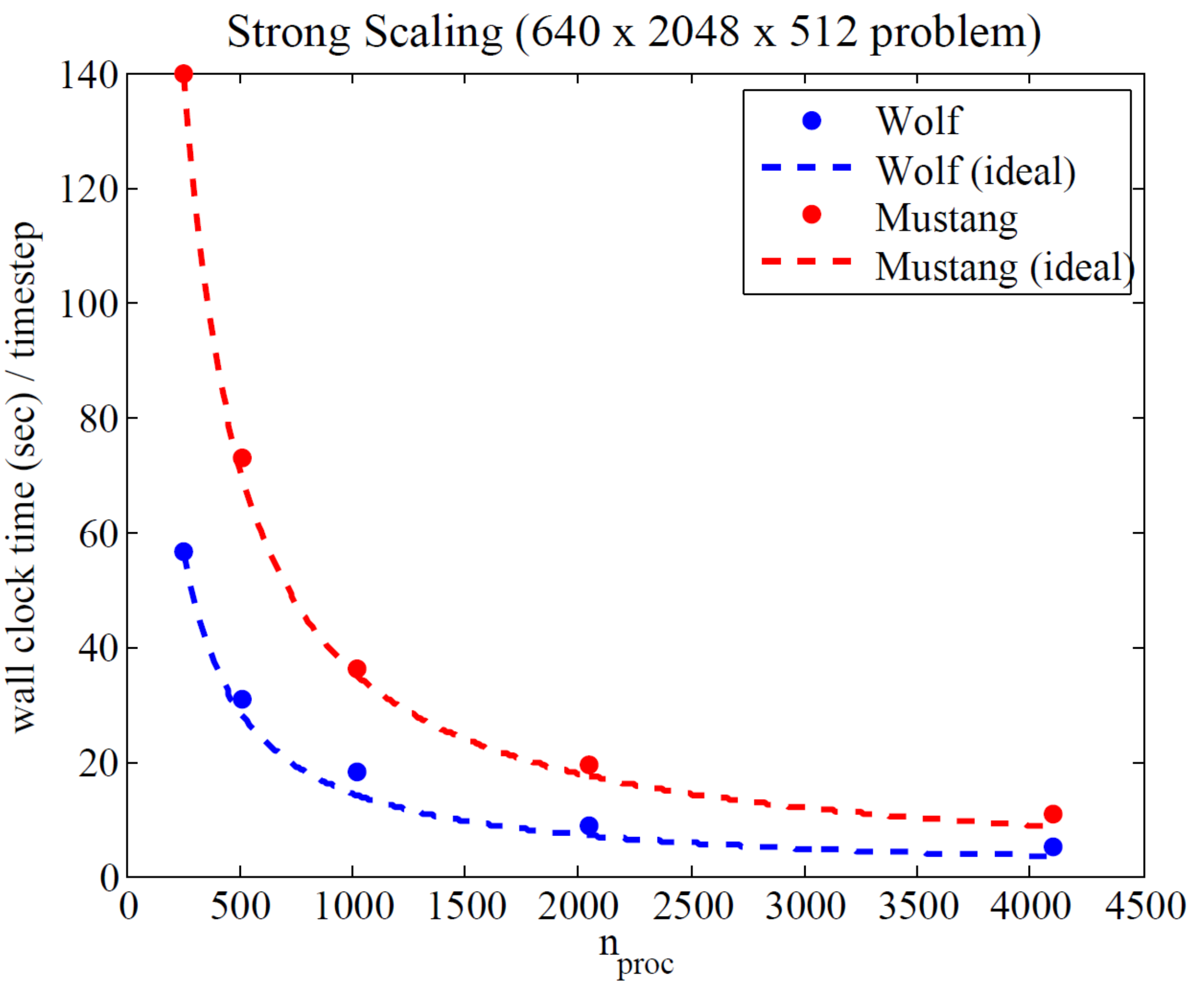


- **Spanwise vorticity (colored by streamwise velocity): structures are often tube-like**



- **From below (lighter-fluid side): coloring reveals that there is a higher concentration of vortices near the free-stream velocity and fewer on the heavier-fluid side**

Performance



Summary

- IC resources are effectively utilized by CFDNS to simulate variable density mixing layers
- Variable density effects in shear flows are important in many practical applications and also for testing multi-material turbulence models